

# Photon-phonon-assisted thermoelectric effects in the molecular devices

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## Abstract

We consider a single level quantum dot interacting with a phonon mode and weakly coupled to metallic leads which are subjected to a time-dependent gate voltage. Electrical conductance, thermopower, and figure of merit are investigated in detail using a Tien-Gordon-type rate equation. In the presence of the microwave field, the electrical conductance exhibits extra peaks whose height is controlled by the magnitude of the microwave field. Furthermore, the oscillation of the thermopower increases in the presence of the time-dependent gate voltage or the electron-phonon interaction. Influence of the electron-phonon interaction, microwave field, temperature, and Coulomb interaction on the figure of merit is also studied.

## 1 Introduction

The study of the thermoelectrical properties of nanoscale devices has attracted a lot of attention in recent years theoretically and experimentally [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. The violation of the Wiedemann Franz law [13, 14], that the ratio of the electrical conductance to the thermal conductance is proportional to the temperature, in nanostructures has caused that the nanostructures have been considered as good candidates for fabricating thermoelectric devices. The thermoelectric efficiency is measured by a dimensionless quantity as figure of merit,  $ZT = S^2 G_e T / (\kappa_e + \kappa_{ph})$  where  $S$  stands for the thermopower and  $G_e$  denotes the electrical conductance.  $\kappa_e$ , and  $\kappa_{ph}$  are the electrical and phononic thermal conductances, respectively. The Coulomb blockade effect [13, 15], discreteness of the energy levels [16], interference effects [10] and so on are the main reasons for high figure of merit in nanoscale devices. The quantum dot (QD) as a promising thermoelectric material has been widely studied during recent years [3, 4, 11, 12, 13, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25].

The influence of the time-dependent gate voltage on the thermoelectric properties and on the heat transport through QD-based devices is a very interesting issue which has been considered very recently. It was predicted that the heat

can be conducted by phonons in the low temperature [26]. In addition, it was reported that the thermopower can be enhanced in the presence of a step-like pulse bias [27, 28]. Pei and co-workers [29] studied the transient heat generation in a QD by applying a step-like pulse bias. They found that the time-dependent bias results in the periodic oscillation of the heat generation. Chi and co-workers [30] studied the thermoelectric properties of a QD in the presence of a microwave field. They reported that the applying microwave leads to the appearance of the extra peaks in the electrical conductance spectrum.

The coupling between the electronic degree of freedom and vibrational degree of freedom or the electron-phonon interaction (EPI) is an important issue in the transport through nanoscale devices resulting in the novel and interesting phenomena. The influence of the EPI on the transport properties of the molecular transistors and the carbon nanotube quantum dots has been extensively studied using both the Keldysh nonequilibrium Green function formalism and the rate equation approach [31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42]. In addition, the thermoelectric properties of the molecular transistors has been analyzed in recent years [12, 43, 44, 45, 46]. However, although the transport properties of such devices has been studied in the presence of the EPI and the time-dependent voltages [47, 48], the influence of the time-dependent gate voltage on the thermoelectric properties of the molecular devices has not been addressed so far. In this article, we consider a molecule attached to the metallic leads which are subjected to a microwave field in the non-adiabatic regime. We follow the method introduced by Dong and co-workers [48] to obtain the formal expressions of the thermopower and electrical conductance. The analytical relations for the thermopower and electrical conductance are obtained using a Tien-Gordon-type rate equation. The influence of the EPI, microwave field, temperature and Coulomb repulsion on the figure of merit is also examined. The model and formalism are presented in the next section. Section 3 is devoted to the numerical results, and in the end, some sentences are given as a summary.

## 2 Model and formalism

We consider a single level QD interacting with a dispersionless optical phonon mode localized in the QD. The QD is weakly coupled to the normal metal electrodes which are subjected to a time-dependent gate voltage. The Hamiltonian describing the whole system is given as

$$H = \sum_{\alpha k \sigma} \varepsilon_{\alpha k \sigma}(t) c_{\alpha k \sigma}^{\dagger} c_{\alpha k \sigma} + \sum_{\sigma} \varepsilon_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow} + \omega a^{\dagger} a + \lambda \sum_{\sigma} [a^{\dagger} + a] n_{\sigma} + \sum_{\alpha k \sigma} [V_{\alpha k \sigma} c_{\alpha k \sigma}^{\dagger} d_{\sigma} + H.c.], \quad (1)$$

where  $c_{\alpha k \sigma}(c_{\alpha k \sigma}^{\dagger})$  destroys (creates) an electron with wave vector  $k$ , spin  $\sigma$  in lead  $\alpha$ .  $\varepsilon_{\alpha k \sigma}(t) = \varepsilon_{\alpha k \sigma}^0 + u_{\alpha} \cos \Omega t$  denotes the energy levels of the leads composed of the rigid shift of the Fermi energies of the leads,  $\varepsilon_{\alpha k \sigma}^0$ , and the time-dependent

energies,  $u_{L(R)} = \pm V_{ac}$  induced by a microwave field with the frequency  $\Omega$  and the magnitude  $V_{ac}$ .  $d_\sigma (d_\sigma^\dagger)$  is the annihilation (creation) operator in the QD and  $n_\sigma = d_\sigma^\dagger d_\sigma$  is the occupation operator.  $U$  denotes the on-site Coulomb repulsion whereas,  $\omega$  is the phonon energy.  $\lambda$  and  $V_{\alpha k \sigma}$  describe the electron-phonon coupling strength and tunneling between the QD and the leads, respectively.

The EPI can be eliminated by using a polaronic transformation [49],  $\tilde{H} = e^S H e^{-S}$  where  $S = \exp((a^\dagger - a) \sum_\sigma n_\sigma)$ . The transformation results in decoupling the electronic and phononic subsystems and the renormalization of the QD energy levels and the Coulomb repulsion. The transformed Hamiltonian is given as

$$\begin{aligned} \tilde{H} = & \sum_{\alpha k \sigma} \varepsilon_{\alpha k \sigma} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} + \sum_{\sigma} \tilde{\varepsilon}_\sigma n_\sigma + \tilde{U} n_\uparrow n_\downarrow \\ & \omega a^\dagger a + \sum_{\alpha k \sigma} [V_{\alpha k \sigma} X c_{\alpha k \sigma}^\dagger d_\sigma + H.c.] \end{aligned} \quad (2)$$

where  $\tilde{\varepsilon}_\sigma = \varepsilon_\sigma - \lambda^2/\omega$ ,  $\tilde{U} = U - 2\lambda^2/\omega$ , and  $X = \exp(-\lambda/\omega(a^\dagger - a))$ . In the following, we use the wide band approximation so that the tunneling rate,  $\Gamma_\sigma^\alpha = \sum_k |V_{\alpha k \sigma}|^2$ , is energy-independent. Because the QD-lead coupling is assumed to be so weak,  $\Gamma_\sigma^\alpha \ll T$ , where  $T$  denotes the temperature, and on the other hand, the frequency of the microwave field is so stronger than the tunneling rate, a Tien-Gordon-type rate equation [48, 50] can be used to describe the behavior of the system. With respect to Eq. (2), the isolated QD can be in the empty state, one-electron state, or doubly occupied state with  $n$  phonons. These states are shown by  $P_N^n$  where  $N$  and  $n$  stand for the number of the electrons and phonons, respectively, and obey the following rate equations:

$$\frac{P_0^n}{dt} = \sum_{\alpha m \sigma} [\Gamma_{\alpha \sigma 0}^{mn} P_\sigma^m - \Gamma_{\alpha 0 \sigma}^{nm} P_0^n] \quad (3a)$$

$$\frac{P_\sigma^n}{dt} = \sum_{\alpha m} [\Gamma_{\alpha 0 \sigma}^{mn} P_0^m + \Gamma_{\alpha 2 \sigma}^{mn} P_2^m - (\Gamma_{\alpha \sigma 0}^{nm} + \Gamma_{\alpha \sigma 2}^{nm}) P_\sigma^n] \quad (3b)$$

$$\frac{P_2^n}{dt} = \sum_{\alpha m \sigma} [\Gamma_{\alpha \sigma 2}^{mn} P_\sigma^m - \Gamma_{\alpha 2 \sigma}^{nm} P_2^n] \quad (3c)$$

where  $\Gamma_{\alpha NM}^{nm}$  describes the transition from N-electron state to M-electron state, while the number of phonons is changed from  $n$  to  $m$ . The transition rates are defined as [48]

$$\begin{aligned} \Gamma_{\alpha NM}^{nm} = & \Gamma_\alpha^\alpha e^{-g^2} g^{2|m-n|} \frac{p!}{q!} (L_p^{|m-n|}(g^2))^2 \sum_{j=-\infty}^{\infty} J_j(u_\alpha/\Omega)^2 \\ & [f_\alpha(\tilde{\varepsilon}_M - \tilde{\varepsilon}_N + (m-n)\omega - j\Omega)\Theta(M-N) + \\ & (1 - f_\alpha(\tilde{\varepsilon}_N - \tilde{\varepsilon}_M + (n-m)\omega - j\Omega))\Theta(N-M)] \end{aligned} \quad (4)$$

where  $g = \lambda/\omega$ ,  $p = \min[m, n]$ ,  $q = \max[n, m]$ , and  $\Theta(x)$  is the Heaviside step function.  $N$  and  $M$  denote the number of the electrons in the QD expressed as

$N = 0$ , empty state,  $N = 1$ ,  $\varepsilon_N = \varepsilon_\sigma$  (single electron state), and  $N = 2$ ,  $\varepsilon_N = \tilde{\varepsilon}_\uparrow + \tilde{\varepsilon}_\downarrow + \tilde{U}$  (two electron state).  $L_p^q(x)$  is the generalized Laguerre polynomial and  $J_j(x)$  is the Bessel function of order  $j$ .  $f_\alpha(x) = (1 + \exp((x - \mu_\alpha)/kT))^{-1}$  is the Fermi distribution function of lead  $\alpha$  and  $\mu_\alpha$  stands for the chemical potential of the lead. Note that the leads are assumed to be the normal metal, therefore, the tunneling rate,  $\Gamma^\alpha$ , is spin-independent.

Solving Eqs. (3) in the steady state ( $dP_N^n/dt = 0$ ), the charge and energy currents are expressed as

$$I^\alpha = -\frac{e}{\hbar} \sum_{\sigma nm} [\Gamma_{\alpha 0 \sigma}^{nm} P_0^n + (\Gamma_{\alpha \sigma 2}^{nm} - \Gamma_{\alpha \sigma 0}^{nm}) P_\sigma^n - \Gamma_{\alpha 2 \sigma}^{nm} P_2^n] \quad (5a)$$

$$Q^\alpha = \frac{1}{\hbar} \sum_{\sigma nm} [\Gamma_{\alpha 0 \sigma}^{Qnm} P_0^n + (\Gamma_{\alpha \sigma 2}^{Qnm} - \Gamma_{\alpha \sigma 0}^{Qnm}) P_\sigma^n - \Gamma_{\alpha 2 \sigma}^{Qnm} P_2^n] \quad (5b)$$

where  $\Gamma_{\alpha NM}^{Qnm}$  describes the energy transported in the tunneling process and expressed as

$$\Gamma_{\alpha NM}^{Qnm} = \Gamma^\alpha e^{-g^2} g^{2|m-n|} \frac{p!}{q!} (L_p^{|m-n|}(g^2))^2 \sum_{j=-\infty}^{\infty} J_j(u_\alpha/\Omega)^2 \quad (6)$$

$$[(\tilde{\varepsilon}_M - \tilde{\varepsilon}_N + (m-n)\omega - j\Omega)f_\alpha(\tilde{\varepsilon}_M - \tilde{\varepsilon}_N + (m-n)\omega - j\Omega)\Theta(M-N) +$$

$$(\tilde{\varepsilon}_N - \tilde{\varepsilon}_M + (n-m)\omega - j\Omega)(1 - f_\alpha(\tilde{\varepsilon}_N - \tilde{\varepsilon}_M + (n-m)\omega - j\Omega))\Theta(N-M)]$$

In the linear response regime, the charge and heat currents are expanded as [49]

$$I^\alpha = G_e \Delta V + G_T \Delta T \quad (7a)$$

$$Q^\alpha = M \Delta V + K \Delta T \quad (7b)$$

where  $G_e$  and  $G_T$  are the electrical conductance and thermal coefficient, respectively. The thermopower is computed as  $S = -\Delta V/\Delta T$  in the limit of zero current. In order to compute the above coefficients, we assume  $T_L = T + \Delta T$ ,  $\mu_L = Ef + e\Delta V$ ,  $\mu_R = Ef$ , and  $T_R = T$  where  $Ef$  denotes the Fermi energy of the leads. By expanding the Fermi function of the left lead according to  $f_L(\varepsilon) = f(\varepsilon) - e\Delta V f'(\varepsilon) - \frac{\Delta T}{T}(\varepsilon - Ef)f'(\varepsilon)$  where  $f'(\varepsilon) = \partial f(\varepsilon)/\partial(\varepsilon)$  and setting  $I^L = 1/2(I^L - I^R)$  and  $Q^L = 1/2(Q^L - Q^R)$ , one can easily obtain the thermoelectric coefficients. For simulation purpose, we set  $\omega = 1$  as the energy unit. The reported value of the phonon energy is varied from  $10\mu eV$  to  $10meV$  in the literatures. In addition, we set  $\kappa_{ph} = 3\kappa_0$  where  $\kappa_0 = \pi^2 k^2/3hT$  is the quantum of thermal conductance [51] and, assume that the energy level of the QD is degenerate.

### 3 Numerical results and discussions

Figs. 1a and 1b describe the electrical conductance as a function of the energy level of the QD and temperature, respectively. As it is expected, the main peaks

of the electrical conductance are located in the resonance energies, i.e.,  $\tilde{\varepsilon} = 0$ , and  $\tilde{\varepsilon} = -\tilde{U}$ . First, we analyze the behavior of  $G_e$  in the absence of the EPI. By applying microwave field the electrical conductance shows extra peaks at the energies  $\tilde{\varepsilon} = \pm n\Omega$ , and  $\tilde{\varepsilon} = -U \pm n\Omega$  where  $n$  is an integer. These side peaks are induced by the photon-assisted tunneling channels. Such result has been recently reported in Ref. [30]. By solving Eqs. (4,7), we have obtained the following analytical relation for the electrical conductance

$$G_e = \frac{e^2}{\hbar} \frac{\Gamma^L}{2kTZ} [(1 + e^{-\varepsilon/kT}) \sum_{n=-\infty}^{\infty} \frac{J_n(u_L/\Omega)^2}{1 + \cosh((Ef + n\Omega - \varepsilon)/kT)} + (e^{-\varepsilon/kT} + e^{-(2\varepsilon+U)/kT}) \sum_{n=-\infty}^{\infty} \frac{J_n(u_L/\Omega)^2}{1 + \cosh((Ef + n\Omega - \varepsilon - U)/kT)}] \quad (8)$$

where  $Z = 1 + 2\exp(-\varepsilon/kT) + \exp(-(2\varepsilon+U)/kT)$  is the partition function and  $J_n(x)$  is the Bessel function of order  $n$ . It is straightforward to show that the electrical conductance obeys the following equation for the case  $V_{ac} = 0$

$$G_e = \frac{e^2}{\hbar} \frac{\Gamma^L}{kTZ} [\frac{1}{1 + e^{\varepsilon/kT}} + \frac{e^{U/kT} + e^{-\varepsilon/kT}}{(1 + e^{(\varepsilon+U)/kT})^2}] \quad (9)$$

that it is in agreement with the results presented in Ref. [43]. According to Eq. (9), the height of the main peaks of the electrical conductance is equal to  $\frac{e^2}{\hbar} \frac{\Gamma^L}{6kT}$  if  $u_L = 0$ . In the presence of the time-dependent voltage, the height of the main peaks decreases proportional to  $J_0(u_L/\Omega)^2$ . Therefore, the ratio of the main peak's height in the case  $u_L \neq 0$  to  $u_L = 0$  can contain the important information about the influence of the time-dependent gate voltage on the energy levels of the electrodes. Moreover, the appearance of the extra peaks in the electrical conductance is explained by Eq. (8). The height of these side peaks is controlled by  $J_n(u_L/\Omega)^2$  so that their height increases with increase of  $u_L$ . The dependence of the electrical conductance on the temperature is strongly dependent on the energy level of the QD, so that the electrical conductance is significantly reduced in the resonance energies with increase of temperature. The behavior of the electrical conductance in the electron-hole symmetry point,  $\tilde{\varepsilon} = -\tilde{U}/2$ , is very interesting. In low temperatures,  $kT \ll U$ , and in the absence of the microwave fields, the electrical conductance is zero because the electrons and holes participate in the current with the same weight. The magnitude of the electrical conductance significantly increases in the presence of the time-dependent voltage. By analyzing Eq. (8) in the low temperature limit, it is found that the electrical conductance is equal to  $\frac{e^2}{\hbar} \frac{\Gamma^L}{8kT} [J_{-1}(u_L/\Omega)^2 + J_1(u_L/\Omega)^2]$  so the magnitude of  $G_e$  is increased with increase of  $u_L$ . The influence of the photons is suppressed in the higher temperatures so that the electrical conductance becomes independent of the photon-assisted channels. In the high temperature, the various electronic states participate in the charge transport through the QD thus, the extra channels induced by photons do not have significant role in the charge transport. Now, we study the effect of the EPI on the electrical conductance. As one expects, the position of the main peaks is now shifted because

of the polaronic shift. It is important to note that the distance between the peaks is controlled by the Coulomb interaction considered to be constant in the article,  $\tilde{U} = 2$ . The height of the peaks is exponentially reduced in the presence of the EPI. A careful analysis reveals that the reduction is proportional to the EPI strength as  $e^{-g^2}$ . Such decrease was also observed in the Kondo regime [52] owing to the existence of factor  $e^{-g^2}$  in the density of the states of the QD. Here, the reduction is caused due to the exponential suppression of the tunneling between the QD and the leads in the presence of the EPI. Results also show that the EPI results in the reduction of the electrical conductance, more specifically, in high temperatures. However, the photon-phonon-assisted electrical conductance is more than the elastic case in low temperatures. The decrease of the phonon-assisted electrical conductance comes from the fact that the electron configurations with few phonons are now partially populated but their participations in the conductance are suppressed by  $|L_{m>0}^n(g^2)|^2$ .

Fig. 2 describes the thermopower as a function of the energy level of the QD. The sawtooth oscillation of the thermopower is risen due to the change of the electron number in the QD. By solving Eqs. (4,7), the following analytical relation for the thermopower is obtained in the case  $\lambda = 0$

$$S = \frac{-e\Gamma^L}{2\hbar kT^2 G_e Z} [(1 + e^{-\varepsilon/kT}) \sum_{n=-\infty}^{\infty} \frac{J_n(u_L/\Omega)^2 (\varepsilon - n\Omega)}{1 + \cosh((Ef + n\Omega - \varepsilon)/kT)} + (e^{-\varepsilon/kT} + e^{-(2\varepsilon+U)/kT}) \sum_{n=-\infty}^{\infty} \frac{J_n(u_L/\Omega)^2 (\varepsilon + U - n\Omega)}{1 + \cosh((Ef + n\Omega - \varepsilon - U)/kT)}] \quad (10)$$

When  $u_L = 0$ , the thermopower has three zeros located in the resonance energies and electron-hole symmetry point. In resonance energies the temperature gradient cannot produce the net current and, as a result, the thermopower becomes zero. In the electron-hole symmetry point, both electrons and holes carry the charge and energy with the same weight. Although they carry the energy in the same direction, they carry the charge in the opposite directions so that no net current is produced. The sign of the thermopower shows the kind of charge participated in the transport so that  $S > 0$  is for holes, while  $S < 0$  is for electrons. In the energies more than the resonance energies electrons injected from the hotter lead (the left lead) create the current, whereas for the right hand side of the electron-hole symmetry point, holes create the current. Such behavior was previously reported for single QD and double quantum dot systems [16, 23, 24]. In the presence of the microwave fields and EPI, the oscillations of the thermopower increase because of the phonon-photon-assisted tunneling channels. However, the magnitude of the thermopower decreases proportional to  $J_n(u_L/\Omega)^2$ . Moreover, oscillations become faster with increase of  $u_L$ , because the energy levels of the leads oscillate faster. The slope of the thermopower is roughly estimated like  $1/T$  which is in agreement with the results presented in Ref. [43] for single molecule devices in the sequential tunneling regime. In the energies near the chemical potential of the leads, the sign of the thermopower changes more because the phonons and photons have more

meaningful role in the charge transport from the leads to the QD.

The dependence of the figure of merit on the energy level of the QD and temperature is shown in figs. 3a and 3b, respectively. The figure of merit is zero in the resonance energies and electron-hole symmetry points because of  $S = 0$ . The EPI and microwave fields result in the reduction of the magnitude of the figure of merit because they modulate the tunneling process between the QD and the electrodes so that the thermopower and electrical conductance decrease. However, the number of peaks of  $ZT$  significantly increases in the presence of the microwave fields or the EPI owing to the photon- or phonon-assisted channels. Indeed, the time-dependent gate voltage results in the increase of the thermoelectric efficiency of the device in energies in which the device cannot work as a thermoelectric device without the microwave fields. The same result was reported by Chi and co-workers [30]. In the low temperatures, the figure of merit has a maximum (fig. 3b) because the Coulomb interaction controls the transport process. With increase of temperature resulting in the reduction of the Coulomb interaction effect, the figure of merit is reduced. The position of the peak is slightly shifted in the presence of the EPI or the microwave fields.

Fig. 4a shows the dependence of  $ZT$  on the strength of the EPI and the magnitude of the microwave field. Results show that applying the microwave can partly compensate the negative effect of the EPI on the figure of merit. It comes from the photon-assisted channels resulting in the increase of the thermopower and electrical conductance even in the presence of the EPI. Therefore, the time-dependent gate voltage can be used to improve the thermoelectric efficiency of the molecular devices in the presence of the EPI. The influence of the Coulomb interaction on the figure of merit is analyzed in fig. 4b. In the range of  $\tilde{U} \cong -2\tilde{\varepsilon}$ , ( $\tilde{\varepsilon} = -0.5$ ),  $ZT$  is zero because of the electron-hole symmetry point. Indeed,  $ZT$  approaches zero when the electrons and holes participate in the charge and energy transport. In the both weak and strong  $Us$ ,  $ZT$  takes the finite values. In these cases, electrons carry the charge and energy through the system because the QD is in the two-electron state or one-electron state, respectively. It is interesting to note that  $ZT$  takes the reasonable values in high  $\lambda$ s only in strong  $Us$ . It comes from the fact that the empty state or two-electron state will be populated in strong  $\lambda$  and nearly weak  $U$ , so that holes can also participate in the transport resulting the decrease of the thermopower. Therefore,  $ZT$  becomes very small in weak  $U$  and strong  $\lambda$ .

## 4 Summary

In this article, we have investigated the thermoelectric properties of the molecular devices in the presence of the time-dependent voltage by means of a Tien-Gordon-type rate equation formalism. Analytical expressions of the thermopower and electrical conductance are obtained. Results show that the microwave field results in the appearance of the extra peaks in the conductance spectrum whose height is controlled by the magnitude of the microwave. Electron-phonon interaction results in the reduction of the figure of merit. However, the microwave

field can slightly compensate the negative effect of the EPI. We also find that the figure of merit takes reasonable values in the strong Coulomb interaction if the EPI is very strong.

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**Figure captions**

Figure 1: Electrical conductance (a) as a function of the energy level of the QD, (b) as a function of temperature. Parameters are  $\Omega = 0.5$ ,  $\Gamma_0 = 0.01\omega$ , and  $\tilde{U} = 2\omega$ .  $kT = 0.1$  in fig. 1a and  $\varepsilon = -\omega$  in fig. 1b.

Figure 2: Thermopower versus the energy level of the QD. Parameters are the same as fig. 1 except  $\tilde{\varepsilon} = -0.5\omega$ .

Figure 3: Dependence of  $ZT$  on (a) energy level of the QD, (b) temperature. Parameters are the same as fig. 1.  $\tilde{\varepsilon} = -0.5\omega$  in fig. 3b.

Figure 4: Color map of  $ZT$ . Parameters are the same as fig. 3.  $V_{ac} = \omega$  in fig. 4b.

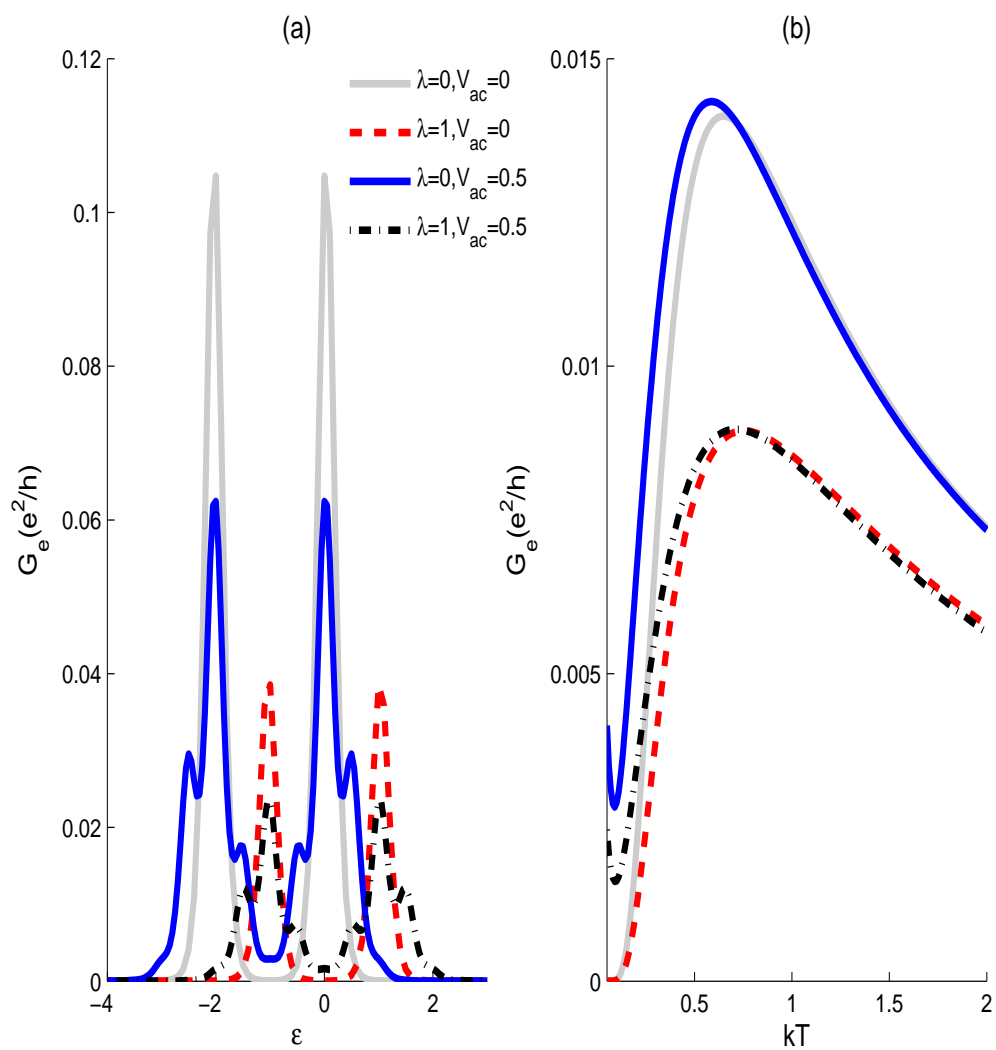


Figure.1

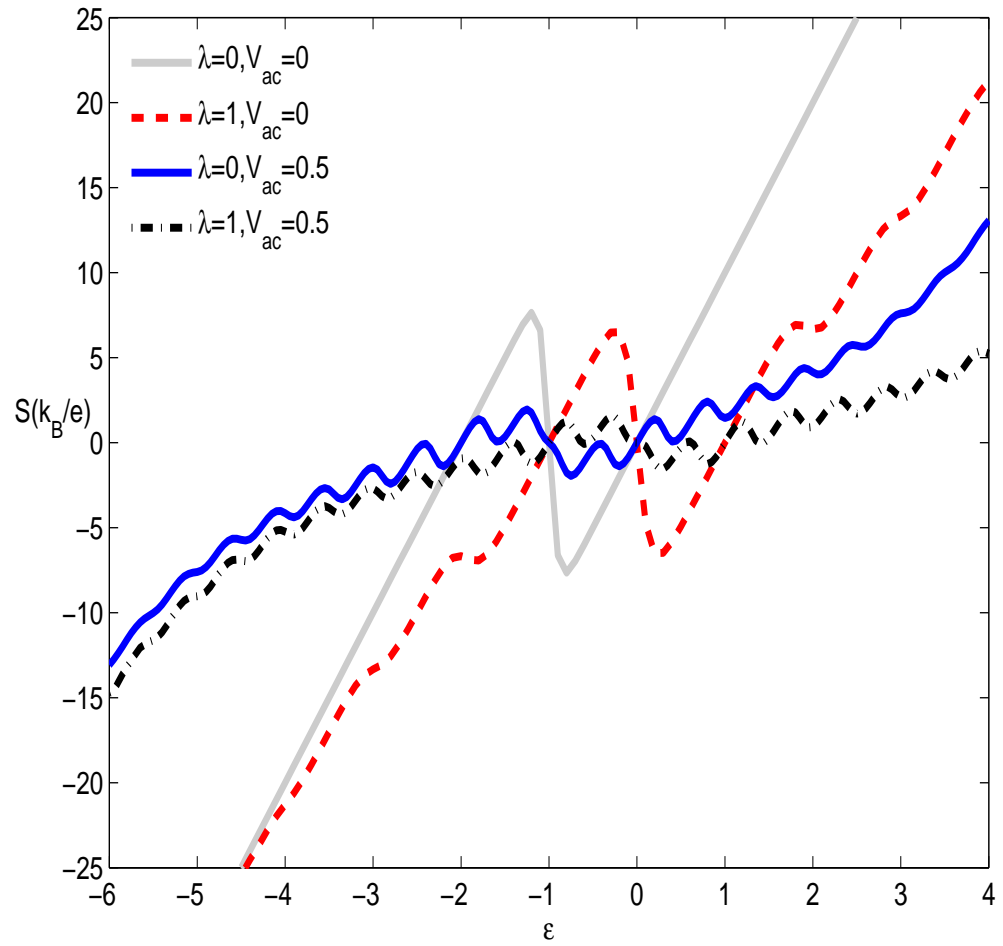


Figure.2

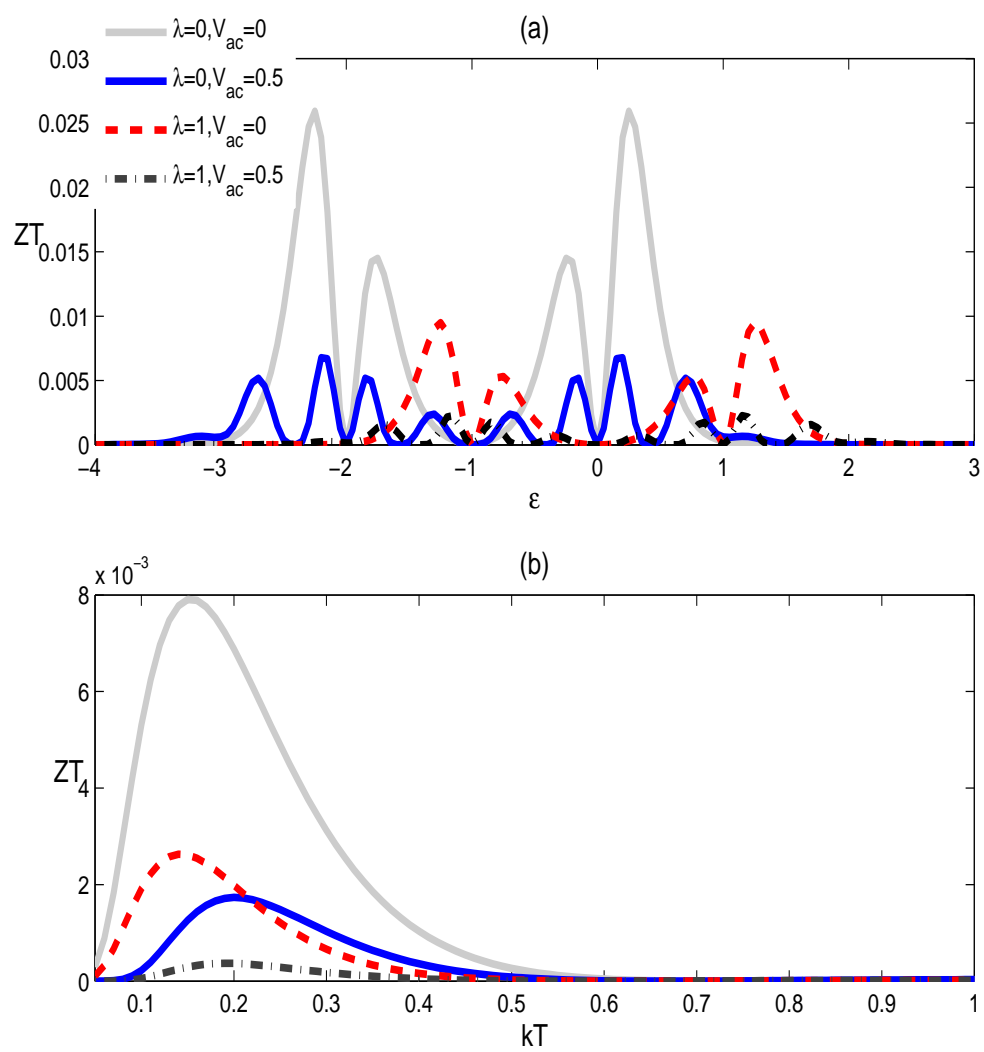


Figure.3

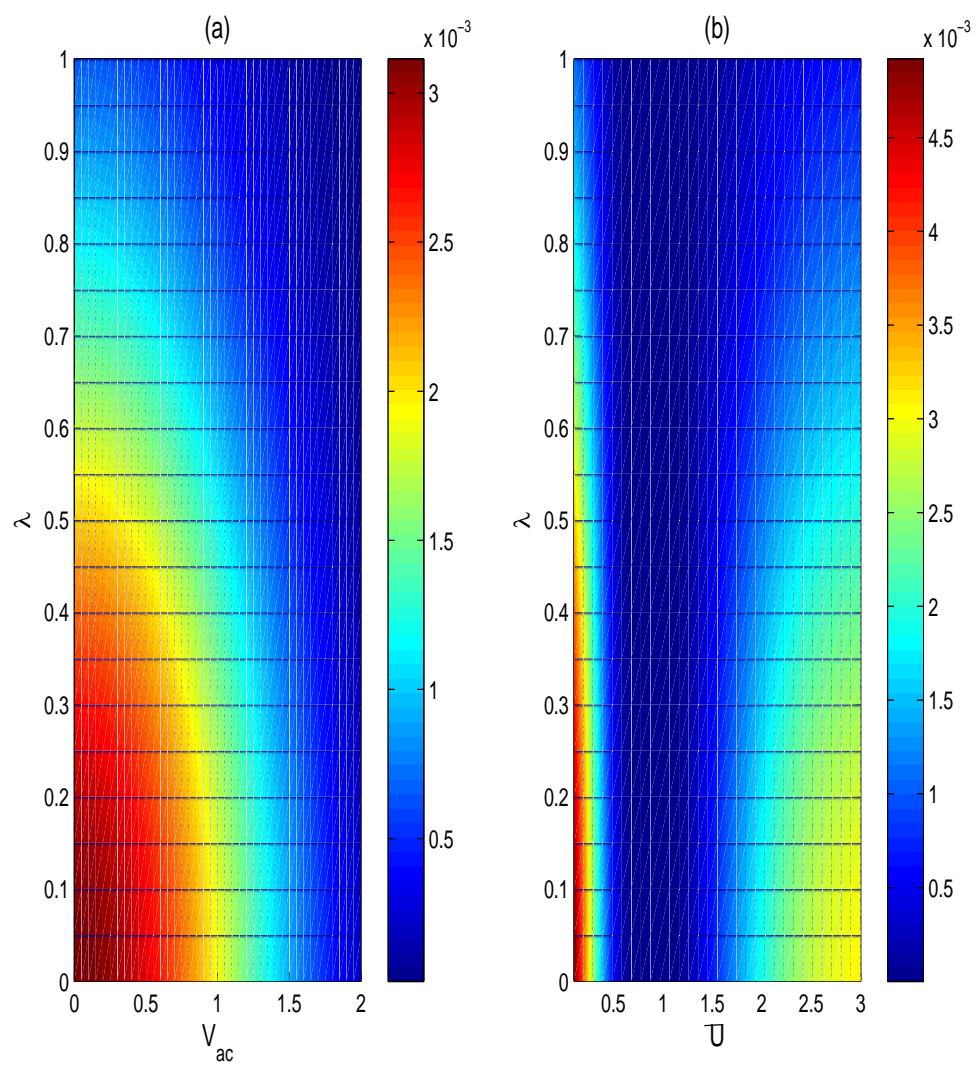


Figure.4